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14. ABSTRACT

This project is focused on reduced basis approximation methods, associated rigorous and sharp *a posteriori* error bounds, and offline-online computational strategies for the rapid and reliable solution of parametrized elliptic, parabolic, and more recently hyperbolic partial differential equations relevant to mechanics from the quantum through the meso-scale to the macro-scale. Typical equations and applications of interest include Density Functional Theory for solid state property calculations, the Boltzmann equation for microscale gas flows, the Navier-Stokes equations for natural convection calculations, elasticity for stress intensity factors/brittle failure, and Helmholtz and the wave equation for acoustic waveguide applications. Of particular interest is real-time and robust parameter estimation with application to detection, nondestructive evaluation, adaptive design/optimization, and control.

In the online/deployed stage, we can provide results for key engineering outputs in *real-time* without loss of accuracy or reliability: the outputs provided — in milliseconds (online) — by our approach are provably indistinguishable from the outputs provided — typically in many minutes or even hours — by classical methods.

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PARAMETER SPACE: THE FINAL FRONTIER

Certified Reduced Basis Methods for
Real-Time Reliable Solution of
Parametrized Partial Differential Equations

FA9550-05-1-0114

Final Report

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March 12, 2007

Abstract

This project is focused on reduced basis approximation methods, associated rigorous and sharp *a posteriori* error bounds, and offline-online computational strategies for the rapid and reliable solution of parametrized elliptic, parabolic, and more recently hyperbolic partial differential equations relevant to mechanics from the quantum through the meso-scale to the macro-scale. Typical equations and applications of interest include Density Functional Theory for solid state property calculations, the Boltzmann equation for microscale gas flows, the Navier-Stokes equations for natural convection calculations, elasticity for stress intensity factors/brittle failure, and Helmholtz and the wave equation for acoustic waveguide applications. Of particular interest is real-time and robust parameter estimation with application to detection, nondestructive evaluation, adaptive design/optimization, and control.

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Our web site `http://augustine.mit.edu/` contains an interactive MATLAB® demo (from the home page click on `worked problems`), as well as a summary of the methodology (from the home page click on `methodology`) and a compendium of our publications (from the `methodology` page click on `Technical Papers`).

Introduction

Engineering analysis requires the prediction of a (or more realistically, several) "output of interest" $s^e \in \mathbb{R}$ — related to energies or forces, stresses or strains, flowrates or pressure drops, temperatures or fluxes, intensities or radar cross-sections — as a function of an "input" parameter P-vector $\mu \in \mathcal{D} \subset \mathbb{R}^P$ — related to geometry, physical

properties, boundary/initial conditions, and loads/sources.

These outputs $s^e(\mu)$ are often functionals of a field variable $u^e(\mu)$,

$$s^e(\mu) = \ell(u^e(\mu); \mu) \; , \tag{1}$$

where $u^e(\mu) \in X^e$ — say displacement, velocity, or current — satisfies a μ-parametrized partial differential equation

$$a(u^e(\mu), v; \mu) = f(v; \mu), \qquad \forall\, v \in X^e \; . \tag{2}$$

Here X^e is the appropriate function space, and a (respectively ℓ, f) are continuous bilinear (respectively, linear) forms. (We consider for simplicity in this brief exposition the linear elliptic case.)

In general, we can not find the exact (our superscript "e" above) solution, and hence we replace $s^e(\mu), u^e(\mu)$ with a (say) Galerkin finite element approximation, $s^{\mathcal{N}}(\mu), u^{\mathcal{N}}(\mu)$: given $\mu \in \mathcal{D}$,

$$s^{\mathcal{N}}(\mu) = \ell(u^{\mathcal{N}}(\mu); \mu) \; , \tag{3}$$

where $u^{\mathcal{N}}(\mu) \in X^{\mathcal{N}}$ satisfies

$$a(u^{\mathcal{N}}(\mu), v; \mu) = f(v; \mu), \qquad \forall\, v \in X^{\mathcal{N}} \; . \tag{4}$$

Here $X^{\mathcal{N}} \subset X^e$ is (say) a standard finite element approximation subspace of dimension $\mathcal{N}$.

Unfortunately, to achieve the desired accuracy, $\mathcal{N}$ must typically be chosen very large; as a result, the evaluation $\mu \to s^{\mathcal{N}}(\mu)$ is simply too costly in the many-query and real-time situations often of interest in engineering. Low-order models — we consider here reduced basis approximations — are thus increasingly popular in the contexts of engineering analysis, parameter estimation, design optimization, and control.

In the reduced basis approach [1, 5, 14, 16], we approximate $s^{\mathcal{N}}(\mu), u^{\mathcal{N}}(\mu)$ — for some fixed sufficiently large "truth" $\mathcal{N} = \mathcal{N}_t$ — with $s_N(\mu), u_N(\mu)$: given $\mu \in \mathcal{D}$,

$$s_N(\mu) = \ell(u_N(\mu); \mu) \; , \tag{5}$$

where $u_N(\mu) \in W_N$ satisfies

$$a(u_N(\mu), v; \mu) = f(v; \mu), \qquad \forall\, v \in W_N \; . \tag{6}$$

(For simplicity here, we consider a purely primal approach; in actual practice, we pursue a primal-dual formulation.)

Here W_N is a problem-specific space of dimension $N \ll \mathcal{N}_t$ which focuses on the (typically very smooth) parametrically induced manifold of interest: $\{u^{\mathcal{N}_t}(\mu) \,|\, \mu \in \mathcal{D}\}$. For example, in the Lagrange reduced basis approach (that we pursue), W_N is the span of snapshots $u^{\mathcal{N}_t}(\mu_n), 1 \le n \le N$, for selected $\mu_n \in \mathcal{D}$; alternatives include the

Taylor, Hermite, and "POD" spaces. Properly selected — as we discuss below — these spaces provide very rapid convergence $u_N(\mu) \to u^{\mathcal{N}_t}(\mu)$ and hence $s_N(\mu) \to s^{\mathcal{N}_t}(\mu)$ as N increases [5, 12].

The dramatic dimension reduction afforded by these reduced basis spaces can be transformed into very significant computational economies: the crucial additional ingredient is an *offline-online computational procedure* [2, 10, 11, 17] that exploits affine or approximate affine parametric structure to greatly reduce the *marginal* cost of each additional output evaluation. This strategy yields very large savings in the many-query and real-time contexts: online (deployed) complexity depends only on N — typically orders of magnitude smaller than $\mathcal{N}_t$ — and *not* on $\mathcal{N}_t$. (Of course, the offline cost remains significant: some of the Accomplishments of this effort address control of the offline computational burden.)

Our focus is the development of *a posteriori* error estimators for reduced basis approximations [11, 13, 17, 20]: inexpensive — *marginal/online complexity independent of* $\mathcal{N}$ — and sharp error bounds $\Delta_N^s(\mu)$ that rigorously bound the error in the output:

$$|s^{\mathcal{N}_t}(\mu) - s_N(\mu)| \leq \Delta_N^s(\mu), \forall\, \mu \in \mathcal{D}\ . \tag{7}$$

Absent such rigorous error bounds we can not determine if N is too small — and our reduced basis approximation unacceptably inaccurate and decision-making compromised — or if N is too large — and our reduced basis approximation unnecessarily expensive and real-time response compromised. In more pragmatic terms, without error bounds we can not rapidly and rigorously determine if critical design or safety conditions and constraints are satisfied: for example, if $s_N(\mu)$ represents a stress intensity factor, does approximate feasibility/safety $s_N(\mu) \leq C$ imply "true" feasibility/safety $s^{\mathcal{N}_t}(\mu) \leq C$? (In the nonlinear context, error bounds are crucial in establishing the very *existence* of a "truth" solution $u^{\mathcal{N}_t}(\mu)$ [9, 19].)

In fact, absent rigorous error bounds, we can not even construct an efficient and well-conditioned reduced basis approximation space W_N. In particular for higher parameter dimensions P, error bounds play a crucial role in "greedy" sampling procedures [7, 8, 13, 20]: we explore a very large subset of the parameter space $\mathcal{D}$ to successively find the points with the largest (inexpensively computed) error *bound*; we only evaluate the truth solution for these winning candidates — the "snapshots" $u^{\mathcal{N}_t}(\mu_n)$ on the parametric manifold the span of which defines W_N. Conventional sampling techniques, which do not exploit error bounds, either can explore only very small subsets of $\mathcal{D}$ or require prohibitively expensive offline effort. Effective sampling procedures are essential to rapid convergence and efficient representation.

Accomplishments

We describe here some specific accomplishments.

a. *Number of parameters.*

We have made considerable progress in at least two directions.

(i) Inf-Sup Lower Bound. We continue to improve the inf-sup lower bound procedure crucial to our *a posteriori* output bounds for difficult (in particular, noncoercive) problems. We can now reasonably treat (say, Helmholtz) problems with several resonances and $O(5)$ parameters. We have developed two approaches.

The first approach is a higher-order expansion based on a new "natural norm." The technique has now been applied in the coercive, non-coercive, and also nonlinear contexts. (See S Sen, K Veroy, DBP Huynh, S Deparis, NC Nguyen, and AT Patera, "Natural norm" *a posteriori* error estimators for reduced basis approximations. Journal of Computational Physics, 217 (1): 37–62, 2006. `doi: j.jcp.2006.02.012`.)

The second approach is a "Successive Constraint Method" which converts the parametric inf-sup lower bound, via a Rayleigh quotient, to a Linear Program. The method offers good theoretical structure, simplicity, and (in tests to date) quite good offline and online performance. Future work is required to develop an *a priori* convergence theory, more efficient constraint selection, and faster Linear Program solution. A paper on this subject has been submitted to CRAS Mathematics (see `http://augustine.mit.edu/methodology/papers/aptCRAS2006preprint.pdf` for the preprint).

(ii) Greedy Sample Selection. On the theoretical front (work with A. Buffa, Y. Maday, C. Prud'homme, G. Turinici), related to approximation, we have shown that *if* a sequence of approximation spaces exist that provide sufficiently rapid (exponential) convergence, then our greedy sample selection procedure will efficiently find an "associated" space that also provides (somewhat less) rapid exponential convergence. Hence although we do not yet know *a priori* when to expect rapid convergence, we do know (roughly) that if *in theory* sufficiently fast exponential convergence is possible, then *in practice* our procedure will also exhibit very good approximation properties. A paper is in preparation.

b. *Generality of parametric dependence.*

We have earlier developed a technique, the "Empirical Interpolation Method" [3], which permits us to develop efficient reduced basis approximations for problems with non-affine parameter dependence [6].

In this project we have developed completely rigorous error estimators for non-affine problems: these estimators rely on a high-order Taylor series development and on the demonstrably rapid convergence of reduced basis approximations for parametric derivatives of the field variable. We have demonstrated the error bounds for several simple model problems. Future work will consider more ambitious problems with non-affine geometric variation.

c. *The Helmholtz equation.*

We have developed reduced basis approximations and *a posteriori* error estimators for

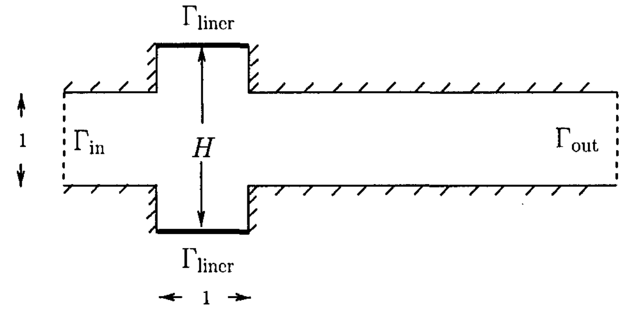

Figure 1: Acoustic Low-Pass Filter Geometry.

waveguides with accurate outflow/radiation conditions for multiple propagating modes (and of course also evanescent modes). These methods will permit us to consider a large range of acoustic waveguide problems related to noise mitigation or detection (say, of buried objects in the seabed).

As an example, we consider here the acoustic low-pass filter waveguide element shown in Figure 1. The parameters are the (non-dimensional) frequency squared, $\mu_1 \equiv k^2$, and the width of the low-pass expansion (relative to the nominal waveguide width), $\mu_2 \equiv H$; we consider the parameter domain $\mu \in \mathcal{D} \equiv [0.1, 5.0] \times [1.75, 2.25]$.

The governing equation is the Helmholtz acoustic equation with inhomogeneous Neumann (imposed velocity) at inflow, Γ_{in}, damping on the liner surface, Γ_{liner}, waveguide radiation/propagation conditions (a Robin condition) on Γ_{out}, and homogeneous Neumann (zero velocity) on all other boundaries.

The output of interest is a transmission coefficient TC, the log of the ratio of the ouput pressure intensity to the input pressure intensity.

We present in Figure 2 the reduced basis output TC_N for $N = 35$ as a function of $\mu_1 \equiv k^2$ at several values of $\mu^2 = H$. We also indicate the error bars: the truth FEM solution will *with certainty* reside within the indicated (rather tight) error bars. For this particular problem the online computational savings — the ratio of the time to calculate the truth output, $s^{\mathcal{N}_t}(\mu)$ to the online time to compute the reduced basis output and error bound, $s_N(\mu)$ and $\Delta_N^s(\mu)$ — is only $O(5)$ rather than the usual $O(100)$ (see e. below and Table 1): first, the truth model for this simple test case is quite coarse; second, the Linear Program performance for our new SCM inf-sup lower bound is quite poor. The latter will be the subject of future work.

We are also collaborating with the group of J. Hesthaven of Brown University and Y. Maday of University of Paris VI on reduced basis methods and *a posteriori* error estimators for electromagnetic Helmholtz applications.

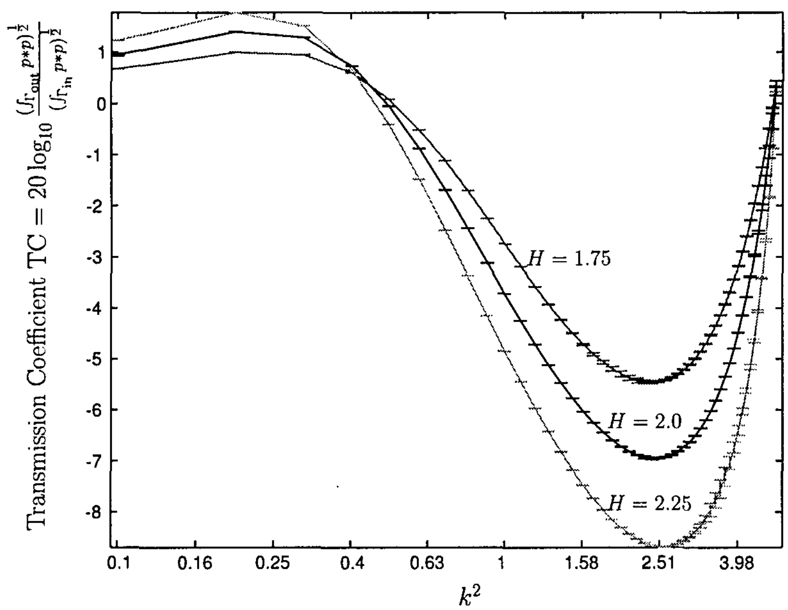

Figure 2: Low-pass filter transmission coefficient as a function of k^2 for different H (see Figurel). As expected, for low k^2 the signal passes; for moderate k^2 the signal is attenuated; and, at higher k^2 (due to harmonics) the signal rebounds.

d. *Real-time robust parameter estimation and uncertainty quantification for detection, adaptive design, and control.*

To date we have further developed our parameter estimation techniques, in particular for the efficient construction of "possibility sets" through application of various optimization procedures. We have also recently discovered that, for an interesting class of elliptic and parabolic problems (e.g., related to transient thermal detection of cracks), we can in fact achieve complete rigor while still maintaining reasonable computational efficiency; the critical enablers are the reduced basis output approximations and *a posteriori* error estimators. A paper has been submitted to the journal *Inverse Problems*.

e. *Stress Intensity Factors.*

Stress Intensity Factors (SIF) are crucial in the prediction of fatigue-induced crack growth and potential brittle failure. In the past, SIF calculations are either too crude (handbooks) or too expensive (direct finite element calculation) to be useful in the most important contexts: many-query evaluation as needed in fatigue studies; real-time evaluation as needed in embedded/health monitoring/lifing analyses.

We have developed a new formulation for SIFs particularly well suited to fast, sharp, and rigorous reduced basis prediction and *a posteriori* error estimation. This new formulation, and associated reduced basis treatment, is described in [8]. This paper also

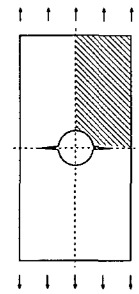

Figure 3: Geometry for Stress Intensity Factor calculation.

N	E_N	$\mathcal{E}_N$	Online Computation Savings
5	1.04E-01	1.66E+02	467
10	6.01E-02	8.72E+01	417
20	9.08E-03	4.39E-01	248
30	2.36E-03	1.31E-01	191
35	9.42E-05	3.17E-02	136
40	4.58E-05	8.86E-03	125

Table 1: Reduced basis error, *a posteriori* error bound, and online computational savings; the latter is the time to compute the truth solution divided by the time to compute (online) the reduced basis output and associated *a posteriori* error bound.

presents several examples, one of which we briefly describe.

We consider here the geometry shown in Figure 3: a pair of symmetric cracks each of length d (measured from the centerline) emanating from a hole of radius R in a (plain strain) specimen of height $2L$; all lengths are non-dimensionalized by the specimen width. Our interest is in the (linear elastic) Stress Intensity Factor, SIF, as a function of our three parameters: $\mu_1 = d$, $\mu_2 = R$, and $\mu_3 = L$. The SIF serves to predict brittle failure, or fatigue-induced crack growth.

We show in Table 1 the error in the reduced basis Energy Release Rate (ERR — the square of the SIF), E_N, the *a posteriori* error bound for the reduced basis prediction, $\mathcal{E}_N$, and the (online) computational savings of the reduced basis approach relative to the FEM truth; the error results reported are the maximum over a large parameter test sample. We observe rapid convergence with N, relatively sharp (and rigorous) error bounds, and very large computational savings.

The reduced basis results can now be used with confidence in predicting failure or crack growth in real-time, a critical capability for component design, health monitoring, and optimal (and safe) mission planning. At present, no other approaches can provide

accurate, real-time, and reliable predictions for critical failure indicators.

Future work will address more complex loadings and geometric configuratons. If successful, our work could replace much of the existing SIF technology.

f. *Hyperbolic problems.*

We have made progress on two classes of hyperbolic problems: first-order wave equations — in particular the Boltzmann equation; and the second-order wave equation — in particular relevant to time-domain acoustics or elastodynamics or Maxwell.

The Boltzmann problem is a very difficult equation that involves independent space and velocity coordinates and (through the collision term) non-local interactions; the equation is increasingly relevant given the growth in microtechnology. We have developed a Petrov Galerkin stabilized formulation of the Boltzmann equation that in turn permits us to develop very rapidly convergent reduced basis approximations and associated rigorous error bounds (e.g., for the flow rate through a microchannel). At present we can consider only one space and velocity coordinate and a simple collision model with two parameters (the Knudsen number and the accommodation coefficient). This work is in collaboration with E. Rønquist; a paper on this topic will appear shortly [15].

For the linear second-order wave equation we have found, perhaps not surprisingly, that for sufficiently smooth initial conditions we can develop rapidly convergent reduced basis approximations. More surprisingly, we have found that we can develop rigorous *a posteriori* error bounds for the error (in the energy norm) as a function of time and parameter. A description of the approach and some first simple numerical tests are provided in [18].

g. *Nonlinear problems.*

We have continued our efforts on the Navier-Stokes equations and natural convection (relevant, for example, to materials processing flows); we are also considering a suite of flows in canonical channel geometries relevant to the design of new microfluidic devices.

On a different front, Density Functional Theory quantum treatment of crystalline (periodic) solid materials, we have recently initiated our first comparisons with conventional (plane wave/Fourier spectral) approaches. It appears that, for our simple model problems, our approaches can significantly reduced the requisite degrees of freedom. This work, in collaboration with Y. Maday, C. Le Bris, and E. Cances, is described in [4].

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Publications

1. K. Veroy and A.T. Patera, Certified real-time solution of the parametrized steady incompressible Navier-Stokes equations; Rigorous reduced-basis *a posteriori* error bounds, *International Journal for Numerical Methods in Fluids*, 47:773–788, 2005.

2. M.A. Grepl and A.T. Patera, *A Posteriori* Error Bounds for Reduced-Basis Approximations of Parametrized Parabolic Partial Differential Equations, *Mathematical Modelling and Numerical Analysis*, 39(1):157–181, 2005.

3. N.C. Nguyen, K. Veroy, and A.T. Patera, Certified Real-Time Solution of Parametrized Partial Differential Equations, in *Handbook of Materials Modeling*, S. Yip (editor), Springer pp. 1523–1558, 2005.

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7. M.A. Grepl, Y. Maday, N.C. Nguyen, and A.T. Patera, Efficient reduced-basis treatment of nonaffine and nonlinear partial differential equations. *Mathematical Modelling and Numerical Analysis*, to appear 2007.

8. É. Cancès, C. Le Bris, Y. Maday, N.C. Nguyen, A.T. Patera, and G.S.H. Pau, Feasibility and competitiveness of a reduced basis approach for rapid electronic structure calculations in quantum chemistry. Proceedings of the Workshop for High-dimensional Partial Differential Equations in Science and Engineering (Montreal), *CRM Proceedings and Lecture Notes*, to appear 2007.

9. A.T. Patera and E. Rønquist, Reduced Basis Approximations and *a posteriori* error estimation for a Boltzmann model. *Computer Methods in Applied Mechanics and Engineering*, to appear 2007.

10. D.B.P. Huynh and A.T. Patera, Reduced basis approximation and a posteriori error estimation for stress intensity factors. *International Journal for Numerical Methods in Fluids*, submitted 2006.

11. D.B.P. Huynh, G. Rozza, S. Sen, and A.T. Patera, A Successive Constraint Linear Optimization Method for Lower Bounds of Parametric Coercivity and Inf-Sup Stability Constants. *CRAS Analyse Numérique*, submitted 2006.

Honors & Awards Received

A.T. Patera, Ford Professor of Engineering, MIT, 2006.

G. Rozza, European Community on Computational Methods in Applied Sciences and Engineering Award for Best Doctoral Thesis, 2006.

G. Rozza, Bill Morton Computational Fluid Dynamics Prize for Young Researchers (under 31 years of age), 2004.